



Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 05:38 AM GMT

PDB ID : 2RGN
Title : Crystal Structure of p63RhoGEF complex with Galpha-q and RhoA
Authors : Shankaranarayanan, A.; Nance, M.R.; Tesmer, J.J.G.
Deposited on : 2007-10-04
Resolution : 3.50 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/XrayValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467
Mogul : 1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix) : 1.9-1692
EDS : rb-20026688
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac : 5.8.0135
CCP4 : 6.5.0
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : trunk26865

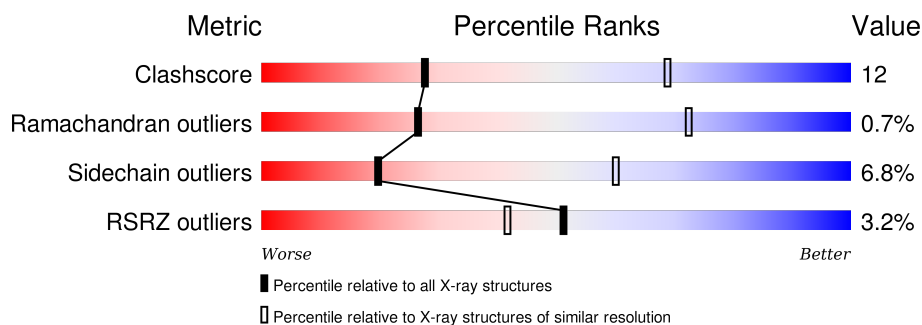
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 3.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
Clashscore	102246	1157 (3.60-3.40)
Ramachandran outliers	100387	1120 (3.60-3.40)
Sidechain outliers	100360	1121 (3.60-3.40)
RSRZ outliers	91569	1058 (3.60-3.40)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	353	<div> <div>0%</div> <div>65%</div> <div>27%</div> <div>8%</div> </div>
1	D	353	<div> <div>2%</div> <div>61%</div> <div>29%</div> <div>8%</div> </div>
2	B	354	<div> <div>3%</div> <div>68%</div> <div>23%</div> <div>8%</div> </div>
2	E	354	<div> <div>3%</div> <div>67%</div> <div>23%</div> <div>8%</div> </div>
3	C	196	<div> <div>7%</div> <div>68%</div> <div>20%</div> <div>10%</div> </div>
3	F	196	<div> <div>4%</div> <div>64%</div> <div>20%</div> <div>14%</div> </div>

2 Entry composition

There are 7 unique types of molecules in this entry. The entry contains 13529 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Guanine nucleotide-binding protein G(q) subunit alpha, Guanine nucleotide-binding protein G(i) subunit alpha-1.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	324	Total	C	N	O	S	0	0	0
			2680	1710	454	504	12			
1	D	324	Total	C	N	O	S	0	0	0
			2680	1710	454	504	12			

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	35	ARG	-	linker	UNP P10824
A	36	SER	-	linker	UNP P10824
D	35	ARG	-	linker	UNP P10824
D	36	SER	-	linker	UNP P10824

- Molecule 2 is a protein called RhoA/RAC/CDC42 exchange factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	327	Total	C	N	O	S	0	0	0
			2677	1697	472	492	16			
2	E	326	Total	C	N	O	S	0	0	0
			2671	1694	471	490	16			

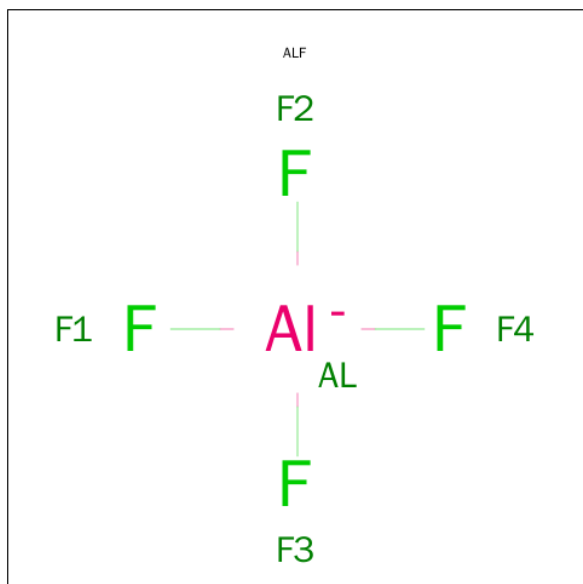
- Molecule 3 is a protein called Transforming protein RhoA.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
3	C	177	Total	C	N	O	S	0	0	0
			1408	891	238	269	10			
3	F	168	Total	C	N	O	S	0	0	0
			1339	847	227	255	10			

There are 6 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
C	-2	GLY	-	expression tag	UNP P61586
C	-1	GLU	-	expression tag	UNP P61586
C	0	PHE	-	expression tag	UNP P61586
F	-2	GLY	-	expression tag	UNP P61586
F	-1	GLU	-	expression tag	UNP P61586
F	0	PHE	-	expression tag	UNP P61586

- Molecule 4 is TETRAFLUOROALUMINATE ION (three-letter code: ALF) (formula: AlF_4).



Mol	Chain	Residues	Atoms			ZeroOcc	AltConf
4	A	1	Total	Al	F	0	0
			5	1	4		
4	D	1	Total	Al	F	0	0
			5	1	4		

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
5	A	1	Total	Mg	0	0
			1	1		
5	D	1	Total	Mg	0	0
			1	1		

- Molecule 6 is GUANOSINE-5'-DIPHOSPHATE (three-letter code: GDP) (formula: $\text{C}_{10}\text{H}_{15}\text{N}_5\text{O}_{11}\text{P}_2$).



Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
6	A	1	Total 28	C 10	N 5	O 11	P 2	0	0
6	D	1	Total 28	C 10	N 5	O 11	P 2	0	0

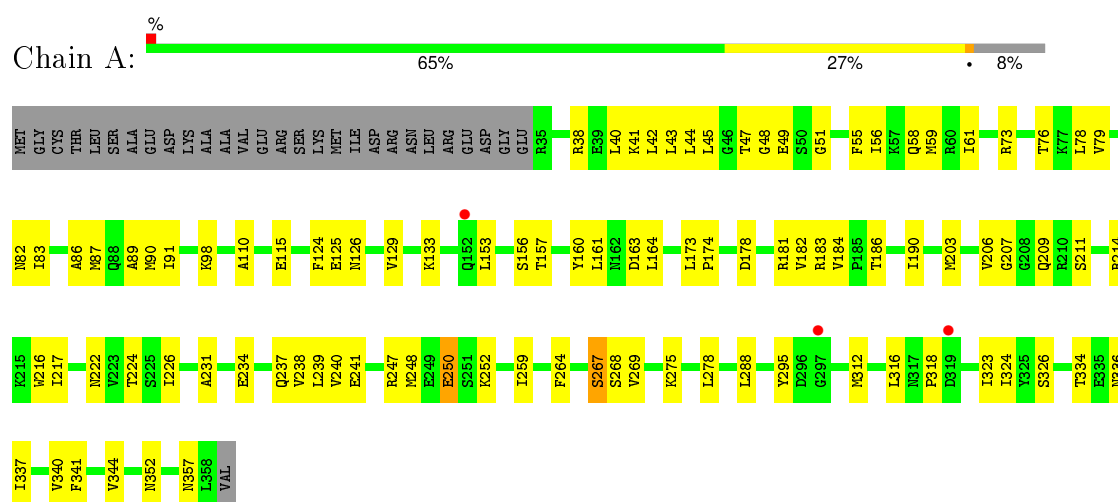
- Molecule 7 is water.

Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
7	A	3	Total O 3 3	0	0
7	D	3	Total O 3 3	0	0

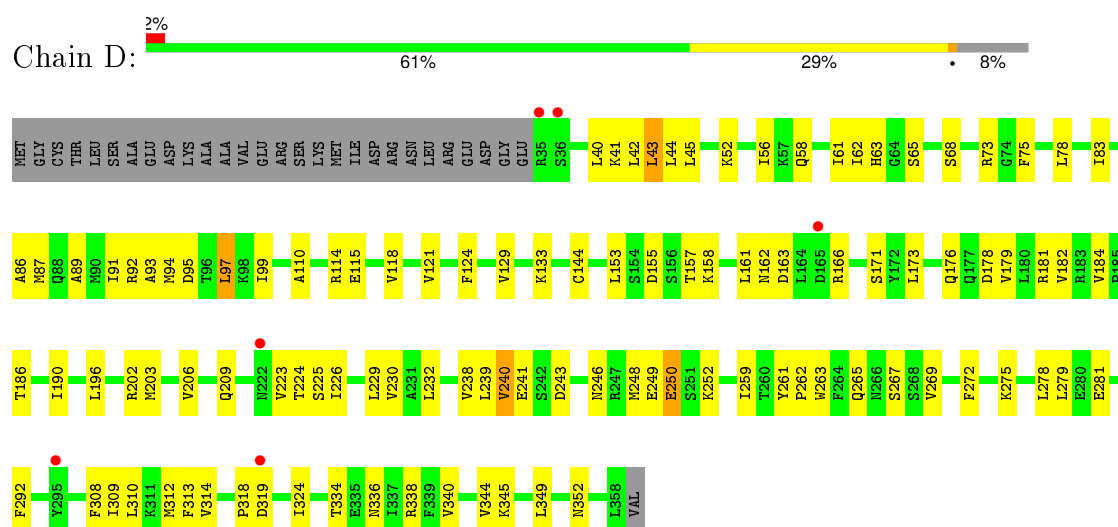
3 Residue-property plots [i](#)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ($RSRZ > 2$). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Guanine nucleotide-binding protein G(q) subunit alpha, Guanine nucleotide-binding protein G(i) subunit alpha-1

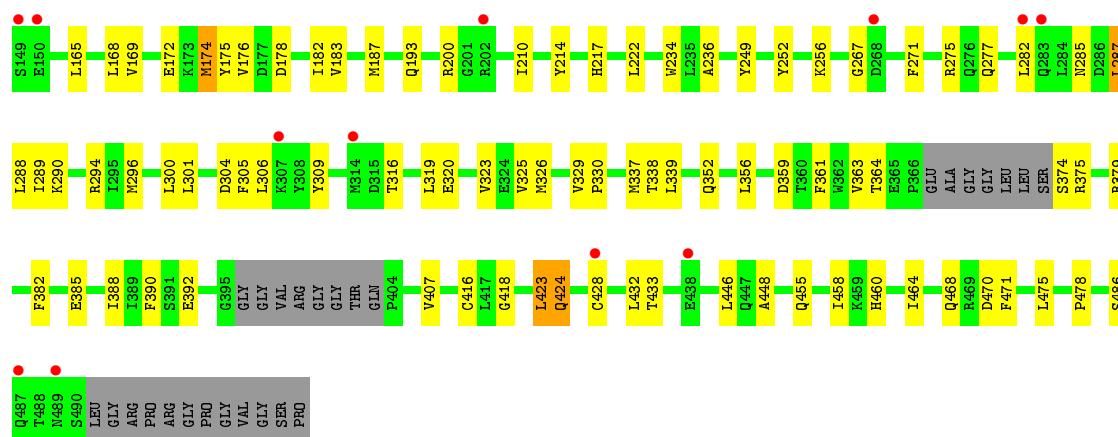


- Molecule 1: Guanine nucleotide-binding protein G(q) subunit alpha, Guanine nucleotide-binding protein G(i) subunit alpha-1

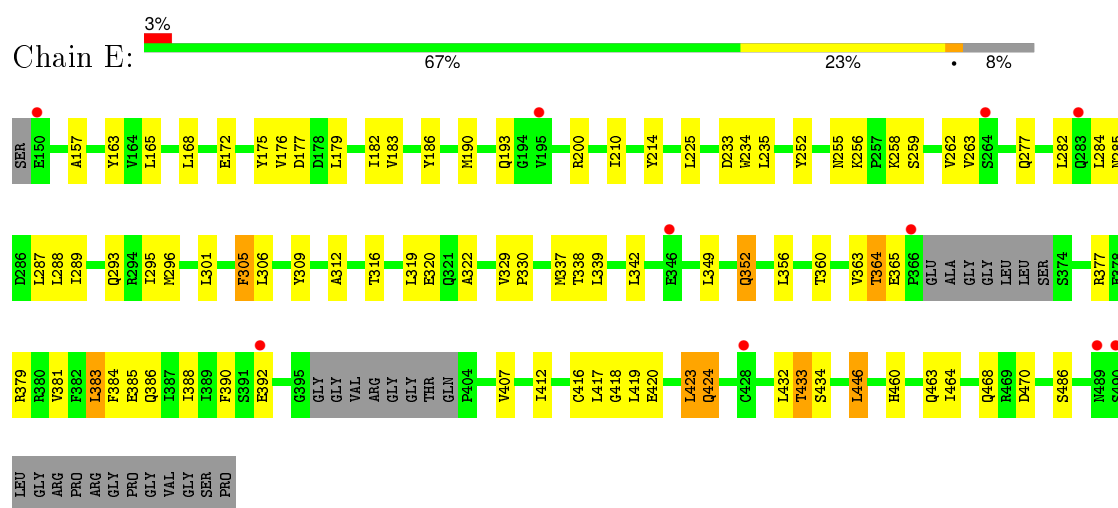


- Molecule 2: RhoA/RAC/CDC42 exchange factor

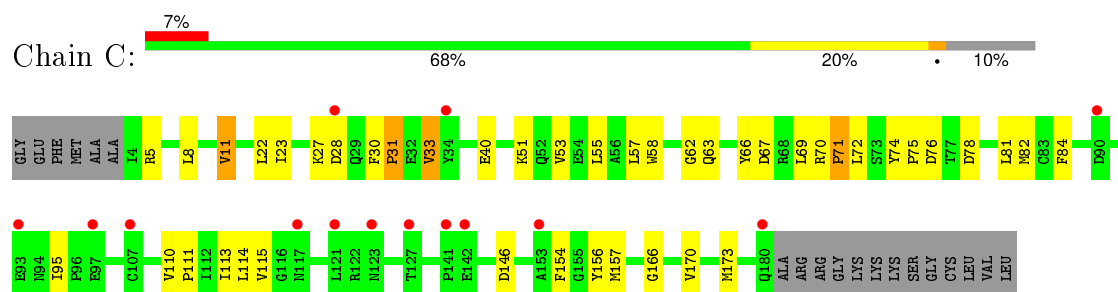




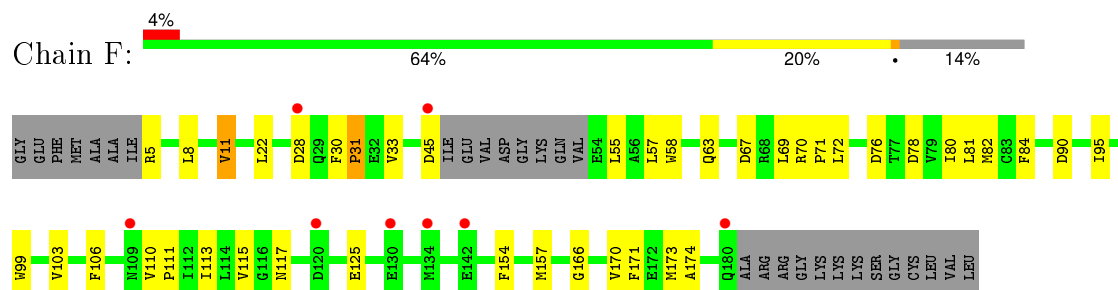
- Molecule 2: RhoA/RAC/CDC42 exchange factor



- Molecule 3: Transforming protein RhoA



- Molecule 3: Transforming protein RhoA



4 Data and refinement statistics

Property	Value	Source
Space group	P 1	Depositor
Cell constants a, b, c, α , β , γ	67.19Å 68.06Å 138.02Å 80.87° 85.16° 87.09°	Depositor
Resolution (Å)	20.00 – 3.50 19.99 – 3.50	Depositor EDS
% Data completeness (in resolution range)	96.4 (20.00-3.50) 91.9 (19.99-3.50)	Depositor EDS
R_{merge}	0.09	Depositor
R_{sym}	0.09	Depositor
$\langle I/\sigma(I) \rangle$ ¹	2.07 (at 3.52Å)	Xtriage
Refinement program	REFMAC 5.2.0019	Depositor
R, R_{free}	0.243 , 0.299 0.233 , (Not available)	Depositor DCC
R_{free} test set	No test flags present.	DCC
Wilson B-factor (Å ²)	102.1	Xtriage
Anisotropy	0.146	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.23 , 123.9	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Outliers	0 of 29080 reflections	Xtriage
F_o, F_c correlation	0.93	EDS
Total number of atoms	13529	wwPDB-VP
Average B, all atoms (Å ²)	144.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 4.64% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GDP, ALF, MG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 5$	RMSZ	$\# Z > 5$
1	A	0.54	0/2737	0.64	0/3698
1	D	0.54	0/2737	0.63	0/3698
2	B	0.49	0/2728	0.59	0/3667
2	E	0.46	0/2722	0.57	0/3659
3	C	0.40	0/1436	0.53	0/1942
3	F	0.38	0/1366	0.52	0/1846
All	All	0.48	0/13726	0.59	0/18510

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2680	0	2645	75	0
1	D	2680	0	2645	69	0
2	B	2677	0	2661	64	0
2	E	2671	0	2656	61	0
3	C	1408	0	1400	39	0
3	F	1339	0	1325	30	0
4	A	5	0	0	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	5	0	0	0	0
5	A	1	0	0	0	0
5	D	1	0	0	0	0
6	A	28	0	12	1	0
6	D	28	0	12	1	0
7	A	3	0	0	0	0
7	D	3	0	0	0	0
All	All	13529	0	13356	316	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 12.

All (316) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:153:LEU:HD11	1:A:157:THR:HG21	1.22	1.09
1:A:153:LEU:CD1	1:A:157:THR:HG21	1.91	1.00
1:A:259:ILE:HD11	1:A:269:VAL:HG11	1.58	0.85
1:A:78:LEU:HD13	1:A:184:VAL:HG21	1.60	0.82
1:D:78:LEU:HD13	1:D:184:VAL:HG21	1.60	0.81
1:A:86:ALA:CB	1:A:157:THR:HG22	2.13	0.79
2:B:236:ALA:HB2	2:B:319:LEU:HD12	1.65	0.78
2:E:305:PHE:HB3	2:E:319:LEU:HD21	1.65	0.78
3:F:8:LEU:HD13	3:F:57:LEU:HD23	1.66	0.78
3:F:166:GLY:O	3:F:170:VAL:HG23	1.87	0.74
3:F:8:LEU:HD12	3:F:55:LEU:HD21	1.69	0.74
3:F:8:LEU:HD11	3:F:81:LEU:HD11	1.71	0.72
2:E:182:ILE:HD12	2:E:288:LEU:CD2	2.20	0.72
1:A:124:PHE:CD1	1:A:129:VAL:HG22	2.25	0.72
1:A:133:LYS:HG3	1:A:164:LEU:HD13	1.72	0.71
1:A:86:ALA:HB1	1:A:157:THR:HG22	1.73	0.71
3:F:11:VAL:HG23	3:F:82:MET:HA	1.71	0.70
1:D:229:LEU:HD23	1:D:272:PHE:HB2	1.73	0.70
1:D:345:LYS:HG2	1:D:349:LEU:HD12	1.73	0.70
2:E:356:LEU:HD21	2:E:385:GLU:HG3	1.75	0.69
2:B:363:VAL:HG22	2:B:446:LEU:HD23	1.74	0.69
1:A:58:GLN:OE1	1:A:334:THR:HG23	1.93	0.68
2:E:182:ILE:HD12	2:E:288:LEU:HD23	1.75	0.68
1:D:52:LYS:HG2	1:D:229:LEU:HD12	1.74	0.68
3:F:113:ILE:HD13	3:F:154:PHE:HB3	1.74	0.68
1:D:240:VAL:HG13	1:D:241:GLU:OE2	1.94	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:83:ILE:HG23	1:A:161:LEU:HD21	1.76	0.67
3:F:157:MET:HB3	3:F:170:VAL:HG22	1.75	0.67
2:B:296:MET:HE3	3:C:66:TYR:CD1	2.30	0.67
2:E:296:MET:HE2	3:F:63:GLN:HA	1.78	0.66
3:F:8:LEU:HD21	3:F:81:LEU:HD12	1.77	0.66
1:A:78:LEU:HD13	1:A:184:VAL:CG2	2.26	0.66
2:E:339:LEU:HG	2:E:349:LEU:HD13	1.79	0.65
2:B:296:MET:HE2	3:C:63:GLN:HA	1.77	0.65
2:B:356:LEU:HD21	2:B:385:GLU:HG3	1.79	0.64
2:E:316:THR:HG22	2:E:320:GLU:HB2	1.79	0.64
1:A:49:GLU:O	1:A:275:LYS:NZ	2.30	0.63
1:D:40:LEU:HD22	1:D:224:THR:HG21	1.79	0.63
1:D:153:LEU:HD11	1:D:157:THR:HG21	1.81	0.63
2:B:418:GLY:HA3	2:B:433:THR:HG22	1.82	0.62
2:E:417:LEU:HD11	2:E:432:LEU:HD22	1.81	0.62
1:D:124:PHE:CD1	1:D:129:VAL:HG22	2.34	0.62
2:E:316:THR:O	2:E:320:GLU:N	2.32	0.62
1:A:86:ALA:HB2	1:A:157:THR:HG22	1.81	0.62
1:D:259:ILE:HD11	1:D:269:VAL:HG11	1.80	0.62
3:C:157:MET:HE2	3:C:157:MET:HA	1.81	0.62
2:E:175:TYR:CZ	2:E:179:LEU:HD11	2.35	0.62
1:A:61:ILE:HG21	1:A:334:THR:HG21	1.82	0.61
1:A:45:LEU:HD22	1:A:216:TRP:CE3	2.35	0.61
1:A:76:THR:HG22	1:A:174:PRO:HD3	1.82	0.61
1:A:45:LEU:HD23	1:A:206:VAL:HG21	1.81	0.61
2:B:182:ILE:HD11	2:B:287:LEU:CB	2.31	0.61
2:B:392:GLU:HB3	2:B:407:VAL:HG22	1.82	0.61
1:A:87:MET:SD	1:A:91:ILE:HD11	2.40	0.60
3:F:81:LEU:HD21	3:F:174:ALA:HB2	1.82	0.60
1:A:86:ALA:O	1:A:89:ALA:HB3	2.00	0.60
1:D:78:LEU:HD13	1:D:184:VAL:CG2	2.31	0.60
2:E:418:GLY:HA3	2:E:433:THR:HG23	1.83	0.60
2:E:183:VAL:HG21	2:E:214:TYR:CD2	2.37	0.60
2:B:455:GLN:HA	2:B:458:ILE:HD12	1.84	0.60
3:C:22:LEU:CD2	3:C:57:LEU:HD22	2.32	0.60
2:E:412:ILE:HG23	2:E:434:SER:HB2	1.84	0.59
2:B:217:HIS:NE2	2:B:249:TYR:OH	2.33	0.59
2:B:337:MET:HE2	3:C:69:LEU:CD2	2.32	0.59
2:B:182:ILE:HD12	2:B:288:LEU:CD2	2.33	0.59
1:D:153:LEU:CD1	1:D:157:THR:HG21	2.32	0.59
3:F:8:LEU:HD11	3:F:81:LEU:CD1	2.32	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:F:8:LEU:HD13	3:F:57:LEU:CD2	2.31	0.58
3:F:113:ILE:HD12	3:F:173:MET:HG2	1.83	0.58
2:B:256:LYS:HE3	2:B:289:ILE:HD13	1.84	0.58
1:A:231:ALA:HB3	1:A:234:GLU:HG3	1.85	0.58
1:A:226:ILE:HD11	1:A:264:PHE:CE2	2.39	0.58
1:D:83:ILE:HG23	1:D:161:LEU:HD21	1.85	0.58
2:B:471:PHE:CZ	2:B:475:LEU:HD21	2.38	0.58
1:D:86:ALA:CB	1:D:157:THR:HG22	2.33	0.57
2:B:330:PRO:HB2	3:C:66:TYR:CE2	2.39	0.57
1:D:336:ASN:O	1:D:340:VAL:HG23	2.05	0.57
1:A:288:LEU:HD23	1:A:295:TYR:CD2	2.39	0.57
1:A:87:MET:HA	1:A:90:MET:HE2	1.87	0.57
1:A:44:LEU:CD1	1:A:56:ILE:HD11	2.35	0.57
2:E:157:ALA:HB3	2:E:312:ALA:HB2	1.87	0.57
2:B:423:LEU:O	2:B:424:GLN:C	2.41	0.57
2:E:282:LEU:HB2	2:E:287:LEU:HD21	1.86	0.56
3:C:8:LEU:HD11	3:C:81:LEU:HD12	1.87	0.56
3:F:30:PHE:CD1	3:F:31:PRO:HD2	2.41	0.56
2:E:423:LEU:O	2:E:424:GLN:C	2.42	0.56
2:B:236:ALA:HB2	2:B:319:LEU:CD1	2.35	0.56
2:B:182:ILE:HD11	2:B:287:LEU:HB2	1.87	0.56
2:E:356:LEU:HD21	2:E:385:GLU:CG	2.35	0.56
1:D:86:ALA:O	1:D:89:ALA:HB3	2.06	0.56
2:E:383:LEU:HA	2:E:388:ILE:HG22	1.88	0.55
3:C:113:ILE:HD13	3:C:154:PHE:HB3	1.87	0.55
1:D:45:LEU:HD23	1:D:206:VAL:HG21	1.87	0.55
1:D:42:LEU:HD12	1:D:203:MET:SD	2.47	0.55
2:B:306:LEU:HD11	2:B:316:THR:HG23	1.88	0.55
2:B:296:MET:CE	3:C:66:TYR:CD1	2.89	0.55
2:B:296:MET:CE	3:C:63:GLN:HA	2.36	0.55
2:B:210:ILE:HD13	2:B:252:TYR:CE1	2.42	0.55
1:A:173:LEU:O	1:A:173:LEU:HD23	2.06	0.55
2:B:182:ILE:HD12	2:B:288:LEU:HD21	1.89	0.55
2:B:300:LEU:HD11	3:C:62:GLY:CA	2.36	0.55
1:D:63:HIS:ND1	1:D:196:LEU:HD13	2.21	0.55
1:A:40:LEU:HD22	1:A:224:THR:HG21	1.88	0.55
1:A:41:LYS:O	1:A:42:LEU:HD23	2.07	0.55
1:D:223:VAL:HG11	1:D:226:ILE:CD1	2.37	0.55
1:D:99:ILE:HD13	1:D:144:CYS:HB2	1.87	0.54
2:E:337:MET:HE2	3:F:72:LEU:HD11	1.88	0.54
2:B:356:LEU:HD21	2:B:385:GLU:CG	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:248:MET:HE1	1:D:309:ILE:CD1	2.38	0.54
2:B:337:MET:HE1	3:C:72:LEU:HD11	1.89	0.54
2:B:418:GLY:CA	2:B:433:THR:HG22	2.38	0.54
3:C:30:PHE:CD1	3:C:31:PRO:HD2	2.43	0.54
2:B:337:MET:CE	3:C:72:LEU:HD11	2.38	0.54
2:E:157:ALA:CB	2:E:312:ALA:HB2	2.38	0.54
2:B:296:MET:HE3	3:C:66:TYR:CG	2.43	0.54
1:A:206:VAL:HG23	1:A:207:GLY:O	2.08	0.54
1:D:86:ALA:HB2	1:D:157:THR:HG22	1.89	0.53
3:C:33:VAL:O	3:C:33:VAL:HG12	2.08	0.53
2:B:325:VAL:HG12	2:B:326:MET:HE2	1.89	0.53
2:B:329:VAL:HB	2:B:330:PRO:HD3	1.91	0.53
2:B:390:PHE:HE2	2:B:446:LEU:HD21	1.72	0.52
3:C:113:ILE:HD12	3:C:173:MET:HG2	1.90	0.52
3:C:8:LEU:HD11	3:C:81:LEU:CD1	2.39	0.52
2:E:165:LEU:HD13	2:E:235:LEU:HD22	1.90	0.52
1:D:62:ILE:HG22	1:D:63:HIS:CD2	2.43	0.52
3:C:166:GLY:O	3:C:170:VAL:HG23	2.09	0.52
1:D:45:LEU:CD2	1:D:206:VAL:HG21	2.40	0.52
1:A:45:LEU:HD12	1:A:226:ILE:HG23	1.91	0.52
3:F:70:ARG:N	3:F:71:PRO:HD2	2.25	0.52
3:F:99:TRP:O	3:F:103:VAL:HG23	2.10	0.52
1:D:83:ILE:HG23	1:D:161:LEU:CD2	2.40	0.52
1:A:336:ASN:O	1:A:340:VAL:HG23	2.10	0.52
1:D:158:LYS:HG2	1:D:162:ASN:ND2	2.25	0.51
2:E:182:ILE:HD12	2:E:288:LEU:HD21	1.92	0.51
1:A:181:ARG:HA	6:A:360:GDP:O2'	2.10	0.51
2:E:388:ILE:HD12	2:E:432:LEU:HD13	1.92	0.51
2:B:339:LEU:HD13	2:B:382:PHE:CZ	2.44	0.51
1:A:252:LYS:NZ	1:A:312:MET:CE	2.73	0.51
2:B:168:LEU:HB2	2:B:301:LEU:HD13	1.92	0.51
3:C:110:VAL:HG13	3:C:111:PRO:HD2	1.92	0.51
1:D:173:LEU:HD23	1:D:173:LEU:O	2.10	0.51
2:B:300:LEU:HD11	3:C:62:GLY:HA3	1.91	0.51
1:D:248:MET:HE2	1:D:292:PHE:HE1	1.76	0.51
2:B:172:GLU:HG3	2:B:222:LEU:HD13	1.93	0.51
1:D:265:GLN:NE2	1:D:319:ASP:OD2	2.44	0.50
2:B:337:MET:HE2	3:C:69:LEU:HD23	1.91	0.50
2:E:418:GLY:CA	2:E:433:THR:HG23	2.40	0.50
2:B:282:LEU:HB2	2:B:287:LEU:HD21	1.93	0.50
1:A:252:LYS:NZ	1:A:312:MET:HE2	2.27	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:175:TYR:CE2	2:B:294:ARG:HG2	2.47	0.49
2:E:383:LEU:HD12	2:E:384:PHE:O	2.12	0.49
1:D:58:GLN:OE1	1:D:334:THR:HG23	2.12	0.49
1:D:223:VAL:HG11	1:D:226:ILE:HD13	1.93	0.49
1:D:43:LEU:HD12	1:D:45:LEU:HD21	1.95	0.49
3:F:115:VAL:HG12	3:F:117:ASN:ND2	2.26	0.49
2:E:306:LEU:HA	2:E:319:LEU:HD23	1.93	0.49
1:D:246:ASN:HB3	1:D:249:GLU:HB2	1.95	0.49
2:B:165:LEU:O	2:B:169:VAL:HG23	2.13	0.49
2:E:329:VAL:HB	2:E:330:PRO:HD3	1.94	0.49
1:D:224:THR:CG2	1:D:352:ASN:HD21	2.26	0.49
1:D:239:LEU:HD11	1:D:250:GLU:OE2	2.13	0.48
2:E:289:ILE:HG22	2:E:293:GLN:HG3	1.94	0.48
1:A:86:ALA:HB1	1:A:157:THR:CG2	2.41	0.48
2:B:182:ILE:HD11	2:B:287:LEU:HB3	1.94	0.48
2:E:356:LEU:HD13	2:E:460:HIS:NE2	2.27	0.48
1:A:240:VAL:HG12	1:A:241:GLU:OE2	2.14	0.48
1:A:264:PHE:HA	1:A:267:SER:OG	2.13	0.48
2:B:339:LEU:HD13	2:B:382:PHE:CE1	2.49	0.48
1:A:252:LYS:HG2	1:A:316:LEU:HD11	1.96	0.48
2:E:168:LEU:HD13	2:E:301:LEU:HD13	1.95	0.48
1:D:248:MET:HE1	1:D:309:ILE:HD13	1.95	0.48
2:E:186:TYR:CD2	2:E:284:LEU:HD13	2.49	0.48
3:F:71:PRO:HG3	3:F:106:PHE:CE2	2.48	0.47
2:E:392:GLU:HB3	2:E:407:VAL:HG22	1.95	0.47
2:B:330:PRO:HB2	3:C:66:TYR:CZ	2.49	0.47
1:A:224:THR:HG23	1:A:352:ASN:HD21	1.79	0.47
1:D:314:VAL:HG13	1:D:324:ILE:CG2	2.44	0.47
1:A:252:LYS:HZ2	1:A:312:MET:HE1	1.80	0.47
1:D:61:ILE:HG21	1:D:334:THR:HG21	1.96	0.47
3:C:11:VAL:HG23	3:C:82:MET:HA	1.97	0.47
1:D:121:VAL:O	1:D:121:VAL:HG12	2.15	0.47
2:E:295:ILE:HG23	2:E:296:MET:HG3	1.97	0.47
2:E:364:THR:HG22	2:E:365:GLU:H	1.80	0.46
2:E:381:VAL:HG22	2:E:390:PHE:CD2	2.50	0.46
2:B:356:LEU:CD1	2:B:464:ILE:HD11	2.46	0.46
1:D:75:PHE:CE2	1:D:179:VAL:HG13	2.50	0.46
3:C:156:TYR:O	3:C:157:MET:HE3	2.16	0.46
1:D:248:MET:HE2	1:D:292:PHE:CE1	2.51	0.46
1:D:263:TRP:CE2	2:E:386:GLN:HG2	2.50	0.46
3:F:8:LEU:HD21	3:F:81:LEU:CD1	2.44	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:168:LEU:HD13	2:E:301:LEU:CD1	2.46	0.46
2:E:383:LEU:HD13	2:E:388:ILE:CG2	2.45	0.46
2:E:172:GLU:HG2	2:E:225:LEU:HD12	1.97	0.46
3:F:22:LEU:CD2	3:F:57:LEU:HD22	2.46	0.46
1:D:259:ILE:CD1	1:D:269:VAL:HG21	2.45	0.46
2:E:256:LYS:HE3	2:E:289:ILE:HD13	1.98	0.46
3:F:110:VAL:HG13	3:F:111:PRO:HD2	1.98	0.46
2:E:419:LEU:HD12	2:E:420:GLU:N	2.31	0.46
1:A:178:ASP:O	1:A:182:VAL:HG13	2.16	0.46
1:A:226:ILE:HD11	1:A:264:PHE:CD2	2.51	0.46
1:A:252:LYS:HZ2	1:A:312:MET:CE	2.28	0.46
3:C:157:MET:HB3	3:C:170:VAL:HG22	1.98	0.45
1:A:240:VAL:CG1	1:A:241:GLU:OE2	2.64	0.45
1:A:59:MET:HE1	1:A:341:PHE:CB	2.45	0.45
2:B:319:LEU:O	2:B:323:VAL:HG23	2.16	0.45
1:D:62:ILE:HD13	1:D:338:ARG:HA	1.98	0.45
1:D:239:LEU:HD11	1:D:250:GLU:CD	2.37	0.45
1:A:156:SER:O	1:A:160:TYR:HD1	1.99	0.45
2:B:236:ALA:CB	2:B:319:LEU:HD12	2.41	0.45
1:A:161:LEU:CD2	1:A:164:LEU:HD21	2.46	0.45
2:E:182:ILE:HD11	2:E:287:LEU:CB	2.46	0.45
3:C:81:LEU:HD23	3:C:113:ILE:HB	1.98	0.45
1:A:45:LEU:HD22	1:A:216:TRP:CZ3	2.52	0.45
1:D:229:LEU:CD2	1:D:272:PHE:HB2	2.44	0.45
2:B:361:PHE:HE2	2:B:448:ALA:HB2	1.80	0.45
1:D:310:LEU:O	1:D:314:VAL:HG23	2.17	0.45
1:A:43:LEU:HD23	1:A:43:LEU:N	2.32	0.45
1:A:352:ASN:OD1	1:A:357:ASN:ND2	2.50	0.45
3:C:70:ARG:N	3:C:71:PRO:HD2	2.32	0.45
2:E:306:LEU:HD13	2:E:319:LEU:HB3	1.99	0.44
2:E:319:LEU:HA	2:E:322:ALA:HB3	1.97	0.44
1:A:133:LYS:CG	1:A:164:LEU:HD13	2.45	0.44
2:E:342:LEU:HD23	2:E:349:LEU:HD11	1.97	0.44
1:A:73:ARG:NE	1:A:173:LEU:HD12	2.32	0.44
1:D:94:MET:CE	1:D:99:ILE:HG22	2.46	0.44
2:E:182:ILE:CD1	2:E:288:LEU:HD23	2.45	0.44
1:D:345:LYS:CG	1:D:349:LEU:HD12	2.43	0.44
1:A:91:ILE:HG23	1:A:110:ALA:HB1	1.98	0.44
2:B:337:MET:CE	3:C:69:LEU:HD23	2.48	0.44
2:E:352:GLN:HA	2:E:352:GLN:HE21	1.83	0.44
2:E:258:LYS:O	2:E:262:VAL:HG23	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:CG2	1:A:324:ILE:N	2.80	0.44
1:D:94:MET:HE3	1:D:99:ILE:HG22	2.00	0.44
3:C:51:LYS:O	3:C:53:VAL:HG23	2.18	0.44
3:C:157:MET:CB	3:C:170:VAL:HG22	2.48	0.44
2:B:306:LEU:HD11	2:B:316:THR:CG2	2.47	0.44
1:A:250:GLU:HG2	2:B:478:PRO:HG2	2.00	0.44
1:A:76:THR:HG22	1:A:174:PRO:CD	2.46	0.44
3:C:8:LEU:HB2	3:C:55:LEU:HD11	2.00	0.44
1:D:239:LEU:HD11	1:D:250:GLU:CG	2.48	0.44
2:B:174:MET:SD	3:C:40:GLU:OE1	2.76	0.44
1:D:44:LEU:HD13	1:D:56:ILE:HD11	2.00	0.43
1:A:259:ILE:CD1	1:A:269:VAL:HG21	2.48	0.43
1:D:93:ALA:O	1:D:97:LEU:HD12	2.18	0.43
1:D:232:LEU:HB3	1:D:279:LEU:HD22	2.00	0.43
1:A:125:GLU:O	1:A:129:VAL:HG23	2.19	0.43
1:D:86:ALA:HB1	1:D:157:THR:HG22	1.99	0.43
1:A:79:VAL:HG13	1:A:160:TYR:CE2	2.54	0.43
1:A:51:GLY:O	1:A:55:PHE:HD1	2.01	0.43
2:B:361:PHE:CB	2:B:446:LEU:HD22	2.49	0.43
1:A:337:ILE:HA	1:A:337:ILE:HD13	1.91	0.43
1:A:49:GLU:HG2	1:A:183:ARG:NH2	2.34	0.43
2:B:178:ASP:O	2:B:287:LEU:HD12	2.19	0.43
2:B:210:ILE:HD13	2:B:252:TYR:CZ	2.54	0.43
1:A:87:MET:HA	1:A:90:MET:CE	2.48	0.43
2:B:193:GLN:NE2	2:B:277:GLN:HE22	2.16	0.43
2:B:289:ILE:HG13	3:C:58:TRP:CH2	2.54	0.42
1:D:45:LEU:HD23	1:D:206:VAL:CG2	2.47	0.42
1:A:224:THR:CG2	1:A:352:ASN:HD21	2.32	0.42
3:F:8:LEU:HD12	3:F:55:LEU:CD2	2.46	0.42
1:A:161:LEU:HD23	1:A:161:LEU:HA	1.78	0.42
3:C:23:ILE:HG23	3:C:27:LYS:NZ	2.34	0.42
1:D:73:ARG:CZ	1:D:173:LEU:HD12	2.50	0.42
1:D:230:VAL:HG21	1:D:313:PHE:CZ	2.54	0.42
1:A:214:ARG:O	1:A:217:ILE:HG22	2.20	0.42
1:D:178:ASP:O	1:D:182:VAL:HG13	2.20	0.42
1:D:41:LYS:O	1:D:42:LEU:HD23	2.19	0.42
2:E:186:TYR:CE2	2:E:284:LEU:HD13	2.54	0.42
2:B:305:PHE:O	2:B:309:TYR:HB3	2.20	0.42
2:B:183:VAL:HG21	2:B:214:TYR:CD2	2.55	0.42
2:B:182:ILE:HD12	2:B:288:LEU:HD23	2.01	0.42
2:E:186:TYR:CG	2:E:284:LEU:HD13	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:E:255:ASN:ND2	2:E:255:ASN:O	2.52	0.42
3:C:84:PHE:HB3	3:C:95:ILE:HD11	2.02	0.42
1:D:87:MET:O	1:D:91:ILE:HG12	2.18	0.42
1:D:261:TYR:HA	1:D:262:PRO:HD3	1.93	0.41
1:A:237:GLN:C	1:A:247:ARG:HG3	2.40	0.41
2:B:356:LEU:HD13	2:B:460:HIS:NE2	2.35	0.41
2:E:172:GLU:O	2:E:176:VAL:HG23	2.21	0.41
2:E:363:VAL:HG22	2:E:446:LEU:HD22	2.01	0.41
2:E:356:LEU:CD1	2:E:464:ILE:HD11	2.50	0.41
2:E:296:MET:HE3	3:F:69:LEU:HD12	2.01	0.41
1:A:206:VAL:HG21	1:A:216:TRP:CE2	2.56	0.41
1:D:61:ILE:HD13	1:D:176:GLN:NE2	2.36	0.41
3:C:114:LEU:HD12	3:C:115:VAL:H	1.85	0.41
2:B:374:SER:O	2:B:375:ARG:HG2	2.21	0.41
1:D:275:LYS:HD3	1:D:278:LEU:HD12	2.03	0.41
1:A:45:LEU:HD23	1:A:206:VAL:CG2	2.48	0.41
2:E:289:ILE:HG13	3:F:58:TRP:CH2	2.55	0.41
2:E:364:THR:HG22	2:E:365:GLU:N	2.34	0.41
1:D:91:ILE:HG23	1:D:110:ALA:HB1	2.01	0.41
1:A:209:GLN:OE1	1:A:209:GLN:N	2.53	0.41
1:D:209:GLN:N	1:D:209:GLN:OE1	2.53	0.41
3:F:171:PHE:HA	3:F:174:ALA:HB3	2.02	0.41
2:B:176:VAL:HG21	2:B:222:LEU:HD22	2.03	0.41
2:B:267:GLY:O	2:B:271:PHE:CD1	2.74	0.41
3:F:84:PHE:HB3	3:F:95:ILE:HD11	2.03	0.41
3:F:70:ARG:N	3:F:71:PRO:CD	2.84	0.41
1:D:308:PHE:CZ	1:D:312:MET:HE3	2.56	0.41
2:E:210:ILE:HD13	2:E:252:TYR:CE1	2.56	0.41
1:D:181:ARG:HA	6:D:360:GDP:O2'	2.21	0.41
2:E:339:LEU:HD21	2:E:384:PHE:HZ	1.86	0.40
1:A:231:ALA:HB1	1:A:275:LYS:HD2	2.03	0.40
3:F:80:ILE:CD1	3:F:103:VAL:HG13	2.50	0.40
2:B:388:ILE:CD1	2:B:432:LEU:HD13	2.51	0.40
3:C:74:TYR:N	3:C:75:PRO:CD	2.84	0.40
1:A:42:LEU:HD12	1:A:203:MET:SD	2.61	0.40
3:F:81:LEU:HD23	3:F:113:ILE:HB	2.03	0.40
1:A:239:LEU:HD11	1:A:250:GLU:CD	2.41	0.40
1:A:126:ASN:O	1:A:126:ASN:CG	2.59	0.40
2:E:193:GLN:NE2	2:E:277:GLN:HE22	2.20	0.40
1:A:47:THR:HG22	1:A:48:GLY:N	2.36	0.40
1:A:275:LYS:HD3	1:A:278:LEU:HD12	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:42:LEU:HD22	1:D:225:SER:HB2	2.02	0.40
3:C:84:PHE:CD1	3:C:114:LEU:HD11	2.55	0.40
2:E:259:SER:O	2:E:263:VAL:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	322/353 (91%)	287 (89%)	34 (11%)	1 (0%)	46	84
1	D	322/353 (91%)	289 (90%)	32 (10%)	1 (0%)	46	84
2	B	321/354 (91%)	294 (92%)	26 (8%)	1 (0%)	46	84
2	E	320/354 (90%)	292 (91%)	27 (8%)	1 (0%)	46	84
3	C	175/196 (89%)	157 (90%)	14 (8%)	4 (2%)	8	48
3	F	164/196 (84%)	149 (91%)	12 (7%)	3 (2%)	11	53
All	All	1624/1806 (90%)	1468 (90%)	145 (9%)	11 (1%)	26	72

All (11) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	C	31	PRO
3	F	31	PRO
1	A	318	PRO
3	C	28	ASP
1	D	318	PRO
3	F	28	ASP
2	B	424	GLN
2	E	424	GLN
3	C	33	VAL

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Mol	Chain	Res	Type
3	C	71	PRO
3	F	33	VAL

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	297/321 (92%)	281 (95%)	16 (5%)	27	67
1	D	297/321 (92%)	272 (92%)	25 (8%)	14	50
2	B	288/304 (95%)	267 (93%)	21 (7%)	17	57
2	E	287/304 (94%)	263 (92%)	24 (8%)	14	50
3	C	156/169 (92%)	150 (96%)	6 (4%)	40	76
3	F	148/169 (88%)	140 (95%)	8 (5%)	27	67
All	All	1473/1588 (93%)	1373 (93%)	100 (7%)	20	60

All (100) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	ARG
1	A	82	ASN
1	A	98	LYS
1	A	115	GLU
1	A	163	ASP
1	A	186	THR
1	A	190	ILE
1	A	211	SER
1	A	222	ASN
1	A	238	VAL
1	A	248	MET
1	A	250	GLU
1	A	267	SER
1	A	268	SER
1	A	326	SER
1	A	344	VAL

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Mol	Chain	Res	Type
2	B	174	MET
2	B	187	MET
2	B	200	ARG
2	B	234	TRP
2	B	275	ARG
2	B	285	ASN
2	B	287	LEU
2	B	290	LYS
2	B	304	ASP
2	B	320	GLU
2	B	338	THR
2	B	352	GLN
2	B	359	ASP
2	B	364	THR
2	B	379	ARG
2	B	416	CYS
2	B	423	LEU
2	B	428	CYS
2	B	468	GLN
2	B	470	ASP
2	B	486	SER
3	C	5	ARG
3	C	11	VAL
3	C	67	ASP
3	C	76	ASP
3	C	78	ASP
3	C	146	ASP
1	D	43	LEU
1	D	65	SER
1	D	68	SER
1	D	92	ARG
1	D	95	ASP
1	D	97	LEU
1	D	114	ARG
1	D	115	GLU
1	D	118	VAL
1	D	133	LYS
1	D	155	ASP
1	D	163	ASP
1	D	166	ARG
1	D	171	SER
1	D	186	THR

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Mol	Chain	Res	Type
1	D	190	ILE
1	D	202	ARG
1	D	238	VAL
1	D	240	VAL
1	D	243	ASP
1	D	250	GLU
1	D	252	LYS
1	D	267	SER
1	D	281	GLU
1	D	344	VAL
2	E	163	TYR
2	E	177	ASP
2	E	190	MET
2	E	200	ARG
2	E	233	ASP
2	E	234	TRP
2	E	285	ASN
2	E	305	PHE
2	E	309	TYR
2	E	338	THR
2	E	352	GLN
2	E	360	THR
2	E	364	THR
2	E	377	ARG
2	E	379	ARG
2	E	383	LEU
2	E	416	CYS
2	E	423	LEU
2	E	433	THR
2	E	446	LEU
2	E	463	GLN
2	E	468	GLN
2	E	470	ASP
2	E	486	SER
3	F	5	ARG
3	F	11	VAL
3	F	45	ASP
3	F	67	ASP
3	F	76	ASP
3	F	78	ASP
3	F	90	ASP
3	F	125	GLU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (31) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	111	GLN
1	A	177	GLN
1	A	222	ASN
1	A	244	ASN
1	A	352	ASN
1	A	357	ASN
2	B	209	ASN
2	B	277	GLN
2	B	352	GLN
2	B	422	ASN
2	B	455	GLN
2	B	468	GLN
3	C	117	ASN
3	C	136	GLN
3	C	149	ASN
1	D	111	GLN
1	D	126	ASN
1	D	162	ASN
1	D	176	GLN
1	D	177	GLN
1	D	265	GLN
2	E	193	GLN
2	E	226	GLN
2	E	277	GLN
2	E	285	ASN
2	E	299	GLN
2	E	352	GLN
3	F	109	ASN
3	F	117	ASN
3	F	136	GLN
3	F	149	ASN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

Of 6 ligands modelled in this entry, 2 are monoatomic - leaving 4 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the chemical component dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
6	GDP	A	360	5,4	23,30,30	1.15	2 (8%)	30,47,47	1.81	6 (20%)
4	ALF	A	361	7,6	0,4,4	0.00	-	0,6,6	0.00	-
6	GDP	D	360	5,4	23,30,30	1.16	3 (13%)	30,47,47	1.82	7 (23%)
4	ALF	D	361	7,6	0,4,4	0.00	-	0,6,6	0.00	-

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
6	GDP	A	360	5,4	-	0/12/32/32	0/3/3/3
4	ALF	A	361	7,6	-	0/0/0/0	0/0/0/0
6	GDP	D	360	5,4	-	0/12/32/32	0/3/3/3
4	ALF	D	361	7,6	-	0/0/0/0	0/0/0/0

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	D	360	GDP	C5-C4	2.42	1.46	1.40
6	D	360	GDP	O4'-C1'	2.68	1.44	1.41
6	A	360	GDP	C5-C4	2.87	1.47	1.40
6	D	360	GDP	C6-C5	3.10	1.47	1.41
6	A	360	GDP	C6-C5	3.27	1.47	1.41

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	360	GDP	C5-C6-N1	-4.34	117.66	123.59
6	A	360	GDP	C5-C6-N1	-3.99	118.13	123.59
6	A	360	GDP	C6-C5-C4	-3.49	116.73	120.90
6	D	360	GDP	N3-C2-N1	-3.34	122.36	127.44
6	A	360	GDP	N3-C2-N1	-3.30	122.42	127.44
6	D	360	GDP	C4-C5-N7	-3.23	106.50	109.48
6	A	360	GDP	C4-C5-N7	-3.06	106.66	109.48
6	D	360	GDP	PA-O3A-PB	-3.06	122.42	132.67
6	D	360	GDP	C6-C5-C4	-2.51	117.90	120.90
6	A	360	GDP	C1'-N9-C4	-2.16	123.68	126.94
6	D	360	GDP	C2'-C1'-N9	2.43	118.01	114.29
6	D	360	GDP	C6-N1-C2	4.53	122.23	115.94
6	A	360	GDP	C6-N1-C2	4.88	122.71	115.94

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
6	A	360	GDP	1	0
6	D	360	GDP	1	0

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2	OWAB(Å ²)	Q<0.9
1	A	324/353 (91%)	-0.14	3 (0%) 85 78	135, 143, 150, 158	0
1	D	324/353 (91%)	-0.04	6 (1%) 70 60	136, 144, 150, 158	0
2	B	327/354 (92%)	0.10	12 (3%) 45 36	138, 145, 150, 157	0
2	E	326/354 (92%)	0.09	10 (3%) 52 43	135, 145, 150, 157	0
3	C	177/196 (90%)	0.43	14 (7%) 15 13	143, 145, 147, 149	0
3	F	168/196 (85%)	0.27	8 (4%) 34 27	143, 146, 147, 149	0
All	All	1646/1806 (91%)	0.08	53 (3%) 51 42	135, 145, 149, 158	0

All (53) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	319	ASP	5.6
3	C	28	ASP	5.5
1	D	222	ASN	5.4
2	E	428	CYS	4.7
2	E	490	SER	4.3
3	F	28	ASP	4.2
3	C	141	PRO	4.0
3	C	123	ASN	4.0
2	B	489	ASN	3.9
2	E	489	ASN	3.8
1	D	35	ARG	3.8
2	B	487	GLN	3.4
1	D	319	ASP	3.3
3	C	142	GLU	3.3
3	C	180	GLN	3.3
3	C	107	CYS	3.3
2	E	195	VAL	3.2
3	F	120	ASP	3.2
2	E	366	PRO	3.1

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Mol	Chain	Res	Type	RSRZ
2	B	314	MET	3.0
2	B	150	GLU	2.9
1	A	297	GLY	2.8
2	B	307	LYS	2.8
2	B	428	CYS	2.7
2	B	283	GLN	2.7
2	E	392	GLU	2.7
3	C	121	LEU	2.6
3	F	130	GLU	2.6
3	F	109	ASN	2.6
2	E	264	SER	2.5
3	C	97	GLU	2.5
3	C	153	ALA	2.5
1	D	165	ASP	2.5
3	F	45	ASP	2.4
3	C	34	TYR	2.4
3	C	93	GLU	2.4
2	B	202	ARG	2.4
3	C	117	ASN	2.3
3	F	142	GLU	2.3
3	C	90	ASP	2.3
2	B	438	GLU	2.3
3	C	127	THR	2.2
1	D	36	SER	2.2
2	B	282	LEU	2.2
2	E	150	GLU	2.2
2	B	149	SER	2.1
3	F	134	MET	2.1
2	E	346	GLU	2.1
2	B	268	ASP	2.1
1	D	295	TYR	2.0
1	A	152	GLN	2.0
2	E	283	GLN	2.0
3	F	180	GLN	2.0

6.2 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

6.3 Carbohydrates [i](#)

There are no carbohydrates in this entry.

6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å ²)	Q<0.9
6	GDP	D	360	28/28	0.82	0.28	0.04	132,135,142,148	0
6	GDP	A	360	28/28	0.84	0.25	-0.24	133,134,139,145	0
4	ALF	A	361	5/5	0.83	0.25	-0.32	152,152,152,153	0
4	ALF	D	361	5/5	0.89	0.15	-1.85	151,152,153,154	0
5	MG	A	362	1/1	0.79	0.12	-2.78	148,148,148,148	0
5	MG	D	362	1/1	0.95	0.06	-	148,148,148,148	0

6.5 Other polymers [i](#)

There are no such residues in this entry.