Full wwPDB X-ray Structure Validation Report (i)

Feb 1, 2016 – 05:20 AM GMT

PDB ID	:	2QA8
Title	:	Crystal Structure of the Estrogen Receptor Alpha Ligand Binding Domain Mutant 537S Complexed with Genistein
Authors	:	Nettles, K.W.; Bruning, J.B.; Nowak, J.; Sharma, S.K.; Hahm, J.B.; Shi, Y.; Kulp, K.; Hochberg, R.B.; Zhou, H.; Katzenellenbogen, J.A.; Katzenellenbogen, B.S.; Kim, Y.; Joachmiak, A.; Greene, G.L.
Deposited on	:	2007-06-14
Resolution	:	1.85 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

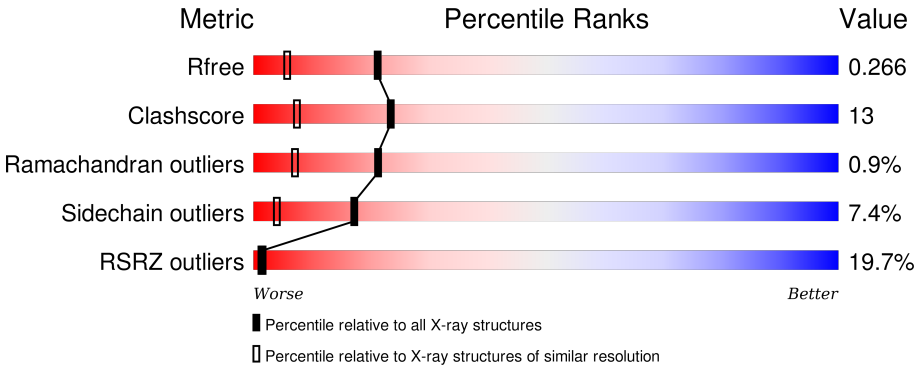
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 1.85 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))
R_{free}	91344	1745 (1.86-1.86)
Clashscore	102246	1898 (1.86-1.86)
Ramachandran outliers	100387	1875 (1.86-1.86)
Sidechain outliers	100360	1875 (1.86-1.86)
RSRZ outliers	91569	1747 (1.86-1.86)

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 <=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	258	13% 72% 14% • 11%
2	B	258	21% 62% 26% • 9%
3	C	13	38% 46% 23% 8% 23%
3	D	13	23% 31% 31% 8% 31%

2 Entry composition

There are 5 unique types of molecules in this entry. The entry contains 4015 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 Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	230	Total	C	N	O	S	0	2	0
			1843	1178	314	330	21			

There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	297	SER	-	CLONING ARTIFACT	UNP P03372
A	530	CME	CYS	MODIFIED RESIDUE	UNP P03372
A	537	SER	TYR	ENGINEERED	UNP P03372

- Molecule 2 is a protein called Estrogen receptor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	235	Total	C	N	O	S	0	4	0
			1894	1215	322	336	21			

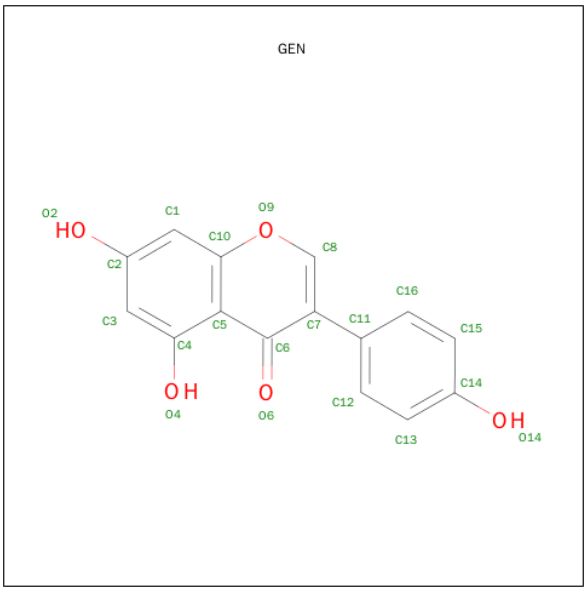
There are 3 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	297	SER	-	CLONING ARTIFACT	UNP P03372
B	381	CME	CYS	MODIFIED RESIDUE	UNP P03372
B	537	SER	TYR	ENGINEERED	UNP P03372

- Molecule 3 is a protein called nuclear receptor coactivator 2.

Mol	Chain	Residues	Atoms				ZeroOcc	AltConf	Trace
3	C	10	Total	C	N	O	0	0	0
			89	57	19	13			
3	D	9	Total	C	N	O	0	0	0
			79	51	16	12			

- Molecule 4 is GENISTEIN (three-letter code: GEN) (formula: $C_{15}H_{10}O_5$).



Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
4	A	1	Total C O 20 15 5	0	0
4	B	1	Total C O 20 15 5	0	0

- Molecule 5 is water.

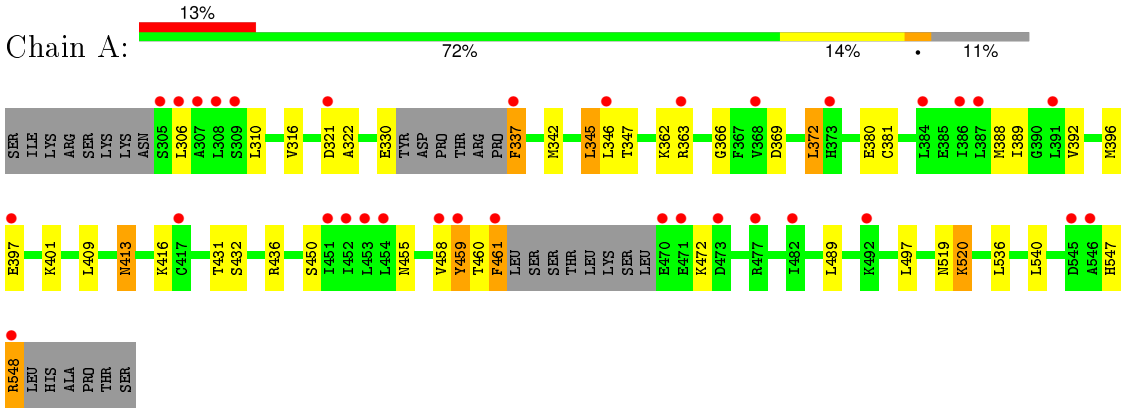
Mol	Chain	Residues	Atoms	ZeroOcc	AltConf
5	A	38	Total O 38 38	0	0
5	B	32	Total O 32 32	0	0

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.

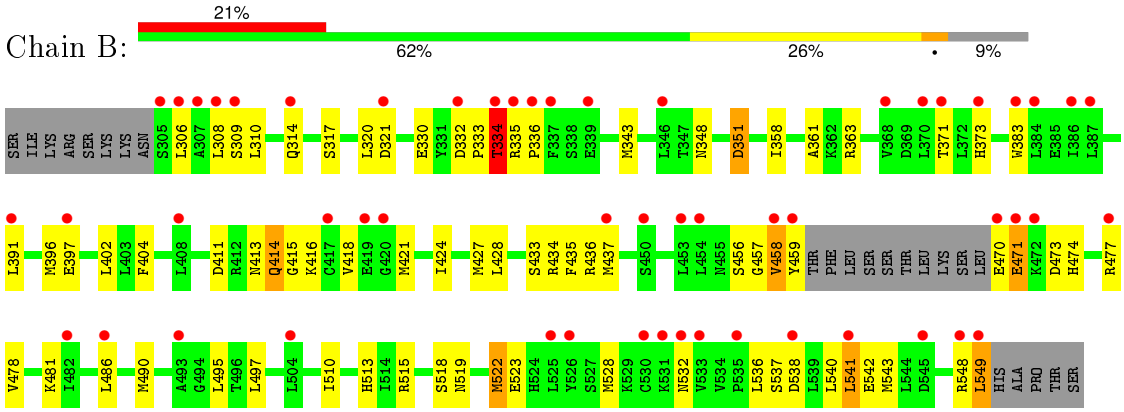
- Molecule 1: Estrogen receptor

Chain A:



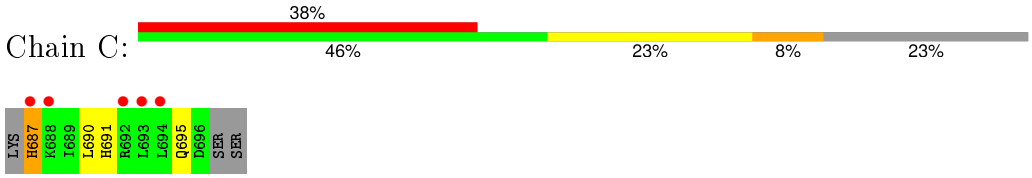
- Molecule 2: Estrogen receptor

Chain B:



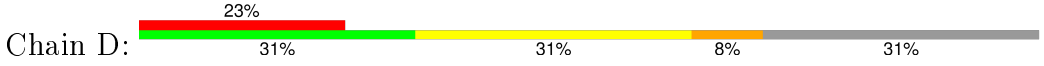
- Molecule 3: nuclear receptor coactivator 2

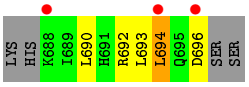
Chain C:



- Molecule 3: nuclear receptor coactivator 2

Chain D:




LYS
HIS
K688
I689
L690
H691
R692
L693
L694
Q695
D696
SER
SER

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	55.67Å 77.96Å 58.00Å 90.00° 109.05° 90.00°	Depositor
Resolution (Å)	19.89 – 1.85 19.89 – 1.85	Depositor EDS
% Data completeness (in resolution range)	96.8 (19.89-1.85) 96.8 (19.89-1.85)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	0.05	Depositor
$< I/\sigma(I) >$ [1]	2.18 (at 1.85Å)	Xtriage
Refinement program	REFMAC 5.2.0005	Depositor
R, R_{free}	0.211 , 0.264 0.211 , 0.266	Depositor DCC
R_{free} test set	1935 reflections (5.29%)	DCC
Wilson B-factor (Å^2)	26.5	Xtriage
Anisotropy	0.237	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.34 , 61.1	EDS
Estimated twinning fraction	0.035 for l,-k,h	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.47$, $< L^2 > = 0.30$	Xtriage
Outliers	0 of 38516 reflections	Xtriage
F_o,F_c correlation	0.94	EDS
Total number of atoms	4015	wwPDB-VP
Average B, all atoms (Å^2)	48.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 7.97% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ 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: CME, GEN

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	0.48	0/1870	0.66	0/2518
2	B	0.43	0/1933	0.60	0/2609
3	C	0.48	0/90	0.61	0/119
3	D	0.36	0/79	0.63	0/104
All	All	0.46	0/3972	0.63	0/5350

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	1843	0	1887	37	0
2	B	1894	0	1953	74	0
3	C	89	0	95	4	0
3	D	79	0	88	4	0
4	A	20	0	8	0	0
4	B	20	0	9	0	0
5	A	38	0	0	1	0
5	B	32	0	0	4	0
All	All	4015	0	4040	106	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 13.

All (106) 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)
2:B:391[B]:LEU:CD1	2:B:402[B]:LEU:HD22	1.57	1.35
1:A:547:HIS:O	1:A:548:ARG:HG3	1.60	1.00
1:A:519:ASN:ND2	2:B:519:ASN:HD22	1.60	1.00
1:A:519:ASN:HD22	2:B:519:ASN:ND2	1.61	0.99
2:B:391[B]:LEU:CD1	2:B:402[B]:LEU:CD2	2.42	0.97
2:B:391[B]:LEU:HD11	2:B:402[B]:LEU:CD2	1.94	0.97
2:B:391[B]:LEU:HD11	2:B:402[B]:LEU:HD22	0.97	0.95
1:A:396:MET:O	1:A:436:ARG:HD3	1.68	0.94
1:A:519:ASN:HD22	2:B:519:ASN:HD22	0.95	0.90
2:B:457:GLY:O	2:B:459:TYR:N	2.08	0.87
2:B:332:ASP:OD2	2:B:334:THR:HG23	1.82	0.80
2:B:351:ASP:OD2	2:B:537:SER:HB2	1.82	0.80
2:B:391[B]:LEU:HD13	2:B:402[B]:LEU:HD22	1.61	0.79
3:C:687:HIS:CE1	3:C:691:HIS:HB3	2.18	0.79
1:A:497:LEU:HD11	2:B:497:LEU:HD11	1.67	0.77
2:B:391[B]:LEU:HD13	2:B:402[B]:LEU:CD2	2.14	0.75
2:B:473:ASP:O	2:B:477:ARG:HG3	1.86	0.74
1:A:372:LEU:HD21	3:C:691:HIS:NE2	2.02	0.74
2:B:413:ASN:HA	2:B:416:LYS:HE3	1.68	0.74
2:B:538:ASP:O	2:B:542:GLU:HG3	1.88	0.73
2:B:411:ASP:H	2:B:414:GLN:HE21	1.34	0.72
1:A:397:GLU:HG2	5:A:605:HOH:O	1.91	0.70
2:B:486:LEU:O	2:B:490:MET:HG3	1.91	0.70
2:B:334:THR:O	2:B:334:THR:OG1	2.09	0.70
1:A:413:ASN:HD22	1:A:416:LYS:NZ	1.90	0.70
2:B:456:SER:HA	2:B:515:ARG:NH2	2.08	0.69
1:A:388:MET:O	1:A:392:VAL:HG12	1.93	0.68
2:B:548:ARG:O	2:B:549:LEU:HB2	1.97	0.65
2:B:309:SER:HB2	5:B:659:HOH:O	1.97	0.64
2:B:396:MET:O	2:B:436:ARG:HD3	1.99	0.63
2:B:333:PRO:O	2:B:335:ARG:N	2.31	0.62
2:B:397:GLU:HG2	5:B:648:HOH:O	1.99	0.62
1:A:459:TYR:CZ	2:B:513:HIS:HB2	2.36	0.60
2:B:434:ARG:HH11	2:B:437:MET:HE3	1.67	0.59
2:B:456:SER:HB2	5:B:635:HOH:O	2.03	0.57
2:B:470:GLU:N	2:B:473:ASP:HB3	2.19	0.57
2:B:433:SER:O	2:B:437:MET:HG3	2.03	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:392:VAL:HG23	1:A:432:SER:CA	2.36	0.56
1:A:459:TYR:CE2	2:B:513:HIS:HB2	2.41	0.55
1:A:413:ASN:HD22	1:A:416:LYS:HZ2	1.52	0.55
1:A:337:PHE:HE1	1:A:345:LEU:CD2	2.20	0.55
2:B:343:MET:HE1	2:B:421:MET:HE2	1.89	0.54
2:B:343:MET:HE1	2:B:421:MET:CE	2.37	0.54
2:B:310:LEU:HD22	2:B:314:GLN:HB3	1.90	0.54
2:B:536:LEU:HB2	2:B:541:LEU:HD13	1.90	0.54
2:B:358:ILE:HD11	3:D:690:LEU:HD12	1.89	0.53
1:A:389:ILE:HA	1:A:392:VAL:CG1	2.39	0.53
2:B:383:TRP:NE1	2:B:543:MET:HB3	2.24	0.52
2:B:358:ILE:HG23	3:D:694:LEU:HD13	1.92	0.52
2:B:434:ARG:HH11	2:B:437:MET:CE	2.23	0.52
2:B:308:LEU:HA	2:B:481:LYS:HD2	1.92	0.52
1:A:401:LYS:HD3	1:A:409:LEU:HG	1.90	0.51
1:A:347:THR:HG21	1:A:536:LEU:CD2	2.41	0.51
2:B:456:SER:HA	2:B:515:ARG:HH22	1.75	0.51
1:A:413:ASN:ND2	1:A:416:LYS:NZ	2.59	0.51
1:A:389:ILE:HA	1:A:392:VAL:HG12	1.91	0.51
2:B:518:SER:O	2:B:522[A]:MET:HG2	2.11	0.50
1:A:392:VAL:HG23	1:A:432:SER:HA	1.94	0.50
2:B:519:ASN:O	2:B:523:GLU:HG2	2.12	0.50
2:B:424:ILE:HA	2:B:427:MET:CE	2.42	0.49
2:B:358:ILE:HD11	3:D:690:LEU:CD1	2.43	0.49
2:B:424:ILE:HA	2:B:427:MET:HE2	1.94	0.49
2:B:330:GLU:HG2	2:B:348:ASN:ND2	2.28	0.49
1:A:372:LEU:HD21	3:C:691:HIS:HE2	1.78	0.49
2:B:474:HIS:O	2:B:478:VAL:HG23	2.13	0.48
2:B:348:ASN:ND2	5:B:613:HOH:O	2.28	0.48
1:A:316:VAL:HG21	1:A:489:LEU:HD21	1.96	0.48
1:A:413:ASN:ND2	1:A:416:LYS:HZ1	2.13	0.47
2:B:343:MET:HE1	2:B:418:VAL:HG11	1.96	0.47
1:A:322:ALA:HB1	1:A:363:ARG:HB2	1.97	0.46
2:B:402[B]:LEU:HD21	2:B:428:LEU:HB3	1.98	0.46
2:B:373:HIS:C	2:B:373:HIS:ND1	2.68	0.46
2:B:435:PHE:HE1	2:B:510:ILE:HG21	1.81	0.45
2:B:343:MET:SD	2:B:528:MET:HG3	2.55	0.45
2:B:371:THR:HG23	2:B:471:GLU:OE1	2.16	0.45
1:A:520:LYS:N	1:A:520:LYS:HD2	2.31	0.45
2:B:537:SER:HB3	2:B:540:LEU:HB2	1.98	0.45
2:B:481:LYS:HE3	2:B:481:LYS:HB3	1.78	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:332:ASP:C	2:B:332:ASP:OD2	2.56	0.44
1:A:392:VAL:HG21	1:A:431:THR:HG22	1.99	0.44
1:A:337:PHE:HE1	1:A:345:LEU:HD22	1.83	0.43
1:A:540:LEU:HA	1:A:540:LEU:HD12	1.76	0.43
2:B:343:MET:CE	2:B:421:MET:HE1	2.49	0.43
2:B:358:ILE:CD1	3:D:690:LEU:HD12	2.48	0.43
2:B:391[A]:LEU:HD13	2:B:404:PHE:HA	2.00	0.43
1:A:459:TYR:C	1:A:461:PHE:H	2.22	0.43
1:A:306:LEU:HD22	1:A:306:LEU:H	1.83	0.43
2:B:458:VAL:O	2:B:458:VAL:HG22	2.19	0.42
2:B:415:GLY:O	2:B:421:MET:HB3	2.19	0.42
2:B:414:GLN:HG2	2:B:414:GLN:H	1.61	0.42
1:A:366:GLY:O	1:A:369:ASP:HB2	2.19	0.42
2:B:361:ALA:C	2:B:363:ARG:N	2.73	0.42
2:B:490:MET:HB3	2:B:495[A]:LEU:HD12	2.02	0.41
1:A:455:ASN:O	1:A:458:VAL:HG12	2.20	0.41
2:B:434:ARG:HD2	2:B:437:MET:HE3	2.02	0.41
1:A:380:GLU:HG3	3:C:690:LEU:HD23	2.02	0.41
2:B:457:GLY:C	2:B:459:TYR:N	2.73	0.41
1:A:458:VAL:HG13	1:A:459:TYR:N	2.36	0.41
2:B:373:HIS:ND1	2:B:373:HIS:O	2.54	0.41
2:B:343:MET:CE	2:B:421:MET:CE	2.99	0.41
1:A:392:VAL:CG2	1:A:432:SER:HA	2.51	0.40
1:A:461:PHE:HB2	1:A:472:LYS:HE3	2.02	0.40
2:B:320:LEU:HA	2:B:320:LEU:HD23	1.90	0.40
2:B:306:LEU:HD13	2:B:306:LEU:HA	1.82	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	224/258 (87%)	222 (99%)	1 (0%)	1 (0%)	39 22
2	B	234/258 (91%)	223 (95%)	8 (3%)	3 (1%)	15 3
3	C	8/13 (62%)	8 (100%)	0	0	100 100
3	D	7/13 (54%)	7 (100%)	0	0	100 100
All	All	473/542 (87%)	460 (97%)	9 (2%)	4 (1%)	21 9

All (4) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	334	THR
2	B	458	VAL
1	A	460	THR
2	B	336	PRO

5.3.2 Protein sidechains (i)

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	207/232 (89%)	190 (92%)	17 (8%)	14 3
2	B	214/232 (92%)	203 (95%)	11 (5%)	29 11
3	C	10/13 (77%)	8 (80%)	2 (20%)	1 0
3	D	9/13 (69%)	5 (56%)	4 (44%)	0 0
All	All	440/490 (90%)	406 (92%)	34 (8%)	17 3

All (34) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	310	LEU
1	A	321	ASP
1	A	330[A]	GLU
1	A	330[B]	GLU
1	A	337	PHE
1	A	342	MET
1	A	345	LEU

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Mol	Chain	Res	Type
1	A	346	LEU
1	A	362	LYS
1	A	372	LEU
1	A	381	CYS
1	A	413	ASN
1	A	450	SER
1	A	459	TYR
1	A	461	PHE
1	A	520	LYS
1	A	548	ARG
2	B	317	SER
2	B	321	ASP
2	B	334	THR
2	B	351	ASP
2	B	414	GLN
2	B	471	GLU
2	B	522[A]	MET
2	B	522[B]	MET
2	B	532	ASN
2	B	541	LEU
2	B	549	LEU
3	C	687	HIS
3	C	695	GLN
3	D	692	ARG
3	D	693	LEU
3	D	694	LEU
3	D	696	ASP

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (12) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	356	HIS
1	A	413	ASN
1	A	455	ASN
1	A	474	HIS
1	A	498	GLN
1	A	519	ASN
2	B	398	HIS
2	B	414	GLN
2	B	513	HIS
2	B	532	ASN
3	C	687	HIS

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Mol	Chain	Res	Type
3	C	695	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

2 non-standard protein/DNA/RNA residues are modelled in this entry.

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	$\#\|Z\| > 2$
1	CME	A	530	1	8,9,10	0.58	0	6,9,11	1.48	1 (16%)
2	CME	B	381	2	8,9,10	0.77	0	6,9,11	1.86	3 (50%)

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
1	CME	A	530	1	-	0/5/8/10	0/0/0/0
2	CME	B	381	2	-	0/5/8/10	0/0/0/0

There are no bond length outliers.

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	381	CME	CZ-CE-SD	-2.84	106.22	113.16
2	B	381	CME	CA-CB-SG	-2.19	106.28	114.23
2	B	381	CME	O-C-CA	-2.07	120.09	125.49
1	A	530	CME	CB-SG-SD	2.09	108.03	103.95

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

2 ligands are modelled in this entry.

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	$\#\|Z\| > 2$
4	GEN	A	600	-	18,22,22	1.82	1 (5%)	23,32,32	0.77	0
4	GEN	B	600	-	18,22,22	1.61	1 (5%)	23,32,32	1.21	2 (8%)

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
4	GEN	A	600	-	-	0/4/4/4	0/3/3/3
4	GEN	B	600	-	-	0/4/4/4	0/3/3/3

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	B	600	GEN	C6-C5	6.22	1.50	1.41
4	A	600	GEN	C6-C5	7.04	1.51	1.41

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	B	600	GEN	C16-C11-C7	-2.52	117.06	120.93
4	B	600	GEN	C7-C6-C5	-2.12	116.98	120.38

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

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, 95^{th} 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	229/258 (88%)	0.90	33 (14%)	3	3	37, 44, 71, 96	0
2	B	234/258 (90%)	1.32	54 (23%)	1	1	35, 45, 77, 97	0
3	C	10/13 (76%)	2.29	5 (50%)	0	0	40, 48, 59, 68	0
3	D	9/13 (69%)	2.04	3 (33%)	0	0	29, 37, 49, 50	0
All	All	482/542 (88%)	1.15	95 (19%)	1	1	29, 45, 74, 97	0

All (95) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	B	549	LEU	12.2
1	A	306	LEU	9.0
2	B	471	GLU	8.2
2	B	535	PRO	7.4
2	B	459	TYR	6.9
2	B	335	ARG	6.5
3	C	687	HIS	6.4
2	B	533	VAL	6.0
2	B	458	VAL	5.9
2	B	470	GLU	5.8
1	A	470	GLU	5.7
2	B	530	CYS	5.6
2	B	532	ASN	5.1
2	B	420	GLY	4.9
1	A	471	GLU	4.7
1	A	459	TYR	4.5
3	D	696	ASP	4.3
2	B	334	THR	4.1
2	B	306	LEU	4.1
2	B	337	PHE	4.1
1	A	482	ILE	3.9

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Mol	Chain	Res	Type	RSRZ
2	B	541	LEU	3.9
2	B	545	ASP	3.8
2	B	336	PRO	3.8
1	A	337	PHE	3.6
3	D	688	LYS	3.5
2	B	493	ALA	3.4
2	B	373	HIS	3.3
2	B	454	LEU	3.3
3	C	688	LYS	3.3
2	B	308	LEU	3.2
1	A	417[A]	CYS	3.2
2	B	371	THR	3.1
1	A	386	ILE	3.0
1	A	368	VAL	3.0
1	A	454	LEU	3.0
2	B	417	CYS	3.0
2	B	531	LYS	2.9
2	B	548	ARG	2.8
2	B	346	LEU	2.8
2	B	307	ALA	2.8
2	B	453	LEU	2.8
3	C	694	LEU	2.8
1	A	548	ARG	2.8
1	A	321	ASP	2.8
2	B	504	LEU	2.8
1	A	452	ILE	2.7
1	A	373	HIS	2.7
2	B	472	LYS	2.6
1	A	461	PHE	2.6
2	B	482	ILE	2.6
2	B	477	ARG	2.6
2	B	383	TRP	2.5
1	A	397	GLU	2.5
2	B	526	TYR	2.5
1	A	346	LEU	2.5
1	A	492	LYS	2.5
1	A	477	ARG	2.5
2	B	305	SER	2.5
2	B	538	ASP	2.5
2	B	397	GLU	2.5
1	A	458	VAL	2.4
1	A	545	ASP	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	308	LEU	2.4
1	A	305	SER	2.4
1	A	453	LEU	2.4
1	A	307	ALA	2.4
1	A	384	LEU	2.3
1	A	387	LEU	2.3
2	B	332	ASP	2.3
1	A	363	ARG	2.3
2	B	525	LEU	2.2
1	A	451	ILE	2.2
2	B	370	LEU	2.2
2	B	408	LEU	2.2
1	A	473	ASP	2.2
2	B	387	LEU	2.2
2	B	384	LEU	2.2
3	C	692	ARG	2.2
2	B	314	GLN	2.2
1	A	391	LEU	2.1
2	B	437	MET	2.1
2	B	368	VAL	2.1
2	B	486	LEU	2.1
2	B	339	GLU	2.1
2	B	386	ILE	2.1
2	B	419	GLU	2.1
1	A	309	SER	2.0
2	B	450	SER	2.0
3	D	694	LEU	2.0
2	B	309	SER	2.0
2	B	391[A]	LEU	2.0
3	C	693	LEU	2.0
1	A	546	ALA	2.0
2	B	321	ASP	2.0

6.2 Non-standard residues in protein, DNA, RNA chains (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, 95^{th} 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
1	CME	A	530	10/11	0.92	0.13	-	33,46,76,78	2
2	CME	B	381	10/11	0.92	0.12	-	39,44,74,76	1

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, 95^{th} 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
4	GEN	A	600	20/20	0.94	0.16	-0.16	16,23,35,37	0
4	GEN	B	600	20/20	0.93	0.13	-1.17	11,30,39,46	0

6.5 Other polymers (i)

There are no such residues in this entry.