



Full wwPDB X-ray Structure Validation Report ⓘ

Aug 20, 2020 – 10:51 PM BST

PDB ID : 6E5V
Title : human mGlu8 receptor amino terminal domain in complex with (S)-3,4-Dicarboxyphenylglycine (DCPG)
Authors : Chen, Q.; Ho, J.D.; Ashok, S.; Vargas, M.C.; Wang, J.; Atwell, S.; Bures, M.; Schkeryantz, J.M.; Monn, J.A.; Hao, J.
Deposited on : 2018-07-23
Resolution : 2.95 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

<https://www.wwpdb.org/validation/2017/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	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.13.1
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.13.1

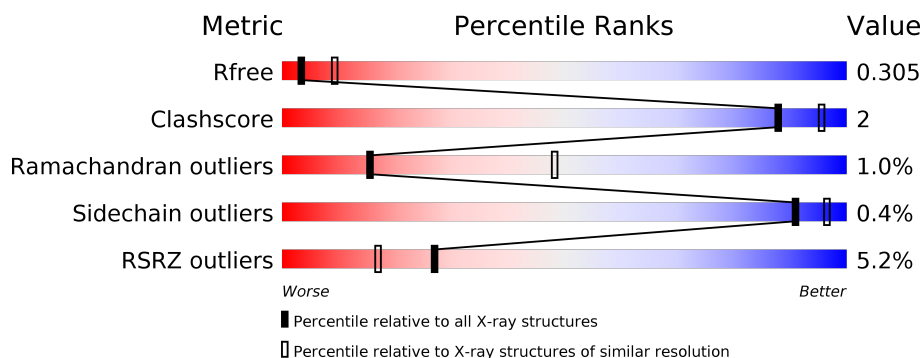
1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

The reported resolution of this entry is 2.95 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}	130704	3104 (3.00-2.92)
Clashscore	141614	3462 (3.00-2.92)
Ramachandran outliers	138981	3340 (3.00-2.92)
Sidechain outliers	138945	3343 (3.00-2.92)
RSRZ outliers	127900	2986 (3.00-2.92)

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 respectively. 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	523	<div> <div>5%</div> <div> <div></div> <div>77%</div> <div>6%</div> <div>17%</div> </div> </div>
1	B	523	<div> <div>4%</div> <div> <div></div> <div>82%</div> <div>•</div> <div>15%</div> </div> </div>

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6754 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 Metabotropic glutamate receptor 8.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	435	Total	C	N	O	S	0	0	0
			3309	2108	559	628	14			
1	B	447	Total	C	N	O	S	0	0	0
			3373	2142	577	640	14			

There are 38 discrepancies between the modelled and reference sequences:

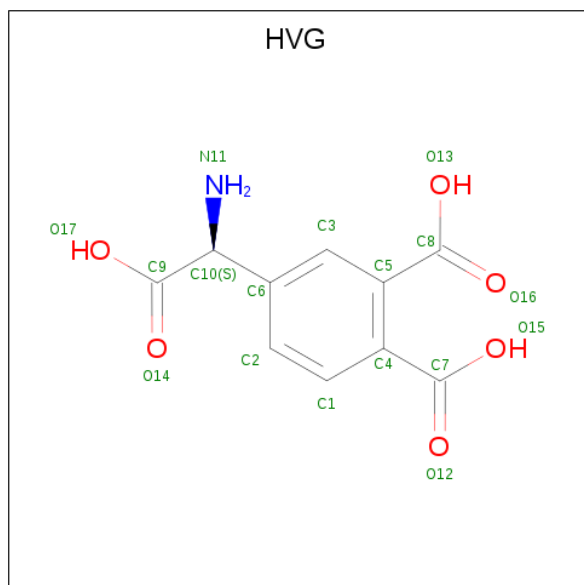
Chain	Residue	Modelled	Actual	Comment	Reference
A	0	MET	-	initiating methionine	UNP O00222
A	1	ALA	-	expression tag	UNP O00222
A	2	LEU	-	expression tag	UNP O00222
A	?	-	GLN	deletion	UNP O00222
A	246	SER	CYS	engineered mutation	UNP O00222
A	509	ASN	-	expression tag	UNP O00222
A	510	LEU	-	expression tag	UNP O00222
A	511	TYR	-	expression tag	UNP O00222
A	512	PHE	-	expression tag	UNP O00222
A	513	GLN	-	expression tag	UNP O00222
A	514	GLY	-	expression tag	UNP O00222
A	515	GLU	-	expression tag	UNP O00222
A	516	GLY	-	expression tag	UNP O00222
A	517	HIS	-	expression tag	UNP O00222
A	518	HIS	-	expression tag	UNP O00222
A	519	HIS	-	expression tag	UNP O00222
A	520	HIS	-	expression tag	UNP O00222
A	521	HIS	-	expression tag	UNP O00222
A	522	HIS	-	expression tag	UNP O00222
B	0	MET	-	initiating methionine	UNP O00222
B	1	ALA	-	expression tag	UNP O00222
B	2	LEU	-	expression tag	UNP O00222
B	?	-	GLN	deletion	UNP O00222
B	246	SER	CYS	engineered mutation	UNP O00222
B	509	ASN	-	expression tag	UNP O00222

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Chain	Residue	Modelled	Actual	Comment	Reference
B	510	LEU	-	expression tag	UNP O00222
B	511	TYR	-	expression tag	UNP O00222
B	512	PHE	-	expression tag	UNP O00222
B	513	GLN	-	expression tag	UNP O00222
B	514	GLY	-	expression tag	UNP O00222
B	515	GLU	-	expression tag	UNP O00222
B	516	GLY	-	expression tag	UNP O00222
B	517	HIS	-	expression tag	UNP O00222
B	518	HIS	-	expression tag	UNP O00222
B	519	HIS	-	expression tag	UNP O00222
B	520	HIS	-	expression tag	UNP O00222
B	521	HIS	-	expression tag	UNP O00222
B	522	HIS	-	expression tag	UNP O00222

- Molecule 2 is 4-[(S)-amino(carboxy)methyl]benzene-1,2-dicarboxylic acid (three-letter code: HVG) (formula: C₁₀H₉NO₆).



Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			17	10	1	6		
2	B	1	Total	C	N	O	0	0
			17	10	1	6		

- Molecule 3 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	B	1	Total 1	Cl 1	0	0
3	A	1	Total 1	Cl 1	0	0

- Molecule 4 is water.

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
4	A	21	Total 21	O 21	0	0
4	B	15	Total 15	O 15	0	0

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes 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.

- Chain A:
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- 5%
- 77%
- 6%
- 17%
- 100
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- CYS
- ARG
- SER
- LEU
- VAL
- MET
- F119
- V120
- Q121
- I124
- GLU
- LYS
- ASP
- ALA
- SER
- ASP
- VAL
- LYS
- CYS
- ALA
- ASN
- GLY
- ASP
- PRO
- ALA
- ILE
- PHE
- THR
- LYS
- P144
- I145
- K146
- I147
- I151
- S156
- T187
- V218
- S223
- Q237
- E241
- I242
- G243
- G244
- P259
- F262
- I265
- V273
- A277
- A282
- T315
- I338
- D339
- G340
- F341
- D342
- R343
- Y344
- E364
- C369
- K370
- L371
- GLY
- SER
- HIS
- GLY
- LYS
- ARG
- ASN
- SER
- HIS
- ILE
- LYS
- LYS
- C384
- T385
- R392
- D393
- V409
- L416
- I428
- S454
- N462
- D466
- I478
- T479
- ASN
- LYS
- S482
- T483
- A505
- HIS
- ARG
- GLU
- ASN
- LEU
- TYR
- PHE
- GLN
- R60
- G61
- V62
- E66
- E77
- I83
- P90
- L93
- S94
- N95
- I96
- V100

- Chain B:
-
- Sequence logo for Chain B. The y-axis represents information content in bits (0.00 to 0.15). The x-axis lists amino acids. A bar chart at the top shows the percentage of conserved residues: 4% (red), 82% (green), and 15% (grey).
- | Position | Amino Acid | Information Content (bits) |
|----------|------------|----------------------------|
| 1 | ASP | 0.01 |
| 2 | PRO | 0.01 |
| 3 | PRO | 0.01 |
| 4 | ILE | 0.01 |
| 5 | PHE | 0.01 |
| 6 | THR | 0.01 |
| 7 | LYS | 0.01 |
| 8 | P144 | 0.01 |
| 9 | S156 | 0.01 |
| 10 | R188 | 0.01 |
| 11 | Y227 | 0.01 |
| 12 | S239 | 0.01 |
| 13 | R240 | 0.01 |
| 14 | GLU | 0.01 |
| 15 | ILE | 0.01 |
| 16 | C243 | 0.01 |
| 17 | S246 | 0.01 |
| 18 | P273 | 0.01 |
| 19 | D274 | 0.01 |
| 20 | A316 | 0.01 |
| 21 | R335 | 0.01 |
| 22 | R343 | 0.01 |
| 23 | C369 | 0.01 |
| 24 | K376 | 0.01 |
| 25 | S379 | 0.01 |
| 26 | H380 | 0.01 |
| 27 | I381 | 0.01 |
| 28 | K382 | 0.01 |
| 29 | L416 | 0.01 |
| 30 | L428 | 0.01 |
| 31 | T436 | 0.01 |
| 32 | L443 | 0.01 |
| 33 | R447 | 0.01 |
| 34 | V449 | 0.01 |
| 35 | M452 | 0.01 |
| 36 | G453 | 0.01 |
| 37 | S454 | 0.01 |
| 38 | G469 | 0.01 |
| 39 | R470 | 0.01 |

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	82.94Å 106.78Å 117.91Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.82 – 2.95 19.82 – 2.95	Depositor EDS
% Data completeness (in resolution range)	98.9 (19.82-2.95) 99.4 (19.82-2.95)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	1.78 (at 2.93Å)	Xtriage
Refinement program	REFMAC 5.8.0103	Depositor
R, R_{free}	0.255 , 0.306 0.255 , 0.305	Depositor DCC
R_{free} test set	1133 reflections (5.06%)	wwPDB-VP
Wilson B-factor (Å ²)	68.6	Xtriage
Anisotropy	0.366	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.29 , 26.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.48$, $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	6754	wwPDB-VP
Average B, all atoms (Å ²)	69.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The analyses of the Patterson function reveals a significant off-origin peak that is 35.02 % of the origin peak, indicating pseudo-translational symmetry. The chance of finding a peak of this or larger height randomly in a structure without pseudo-translational symmetry is equal to 6.2298e-04. The detected translational NCS is most likely also responsible for the elevated intensity ratio.*

¹Intensities estimated from amplitudes.

²Theoretical values of $\langle |L| \rangle$, $\langle L^2 \rangle$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: HVG, CL

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	0.39	0/3380	0.56	0/4593
1	B	0.40	0/3444	0.56	0/4678
All	All	0.40	0/6824	0.56	0/9271

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	3309	0	3160	16	0
1	B	3373	0	3192	10	0
2	A	17	0	0	2	0
2	B	17	0	0	5	0
3	A	1	0	0	0	0
3	B	1	0	0	0	0
4	A	21	0	0	0	0
4	B	15	0	0	0	0
All	All	6754	0	6352	26	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 2.

All (26) 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:B:156:SER:OG	2:B:601:HVG:O14	2.10	0.68
1:A:156:SER:OG	2:A:601:HVG:O14	2.10	0.64
1:A:83:ILE:HD13	1:A:100:VAL:HG22	1.82	0.62
1:B:227:TYR:CE1	2:B:601:HVG:N11	2.72	0.58
1:A:151:ILE:HD13	1:A:409:VAL:HG22	1.90	0.53
1:B:46:ILE:HD13	1:B:416:LEU:HD22	1.93	0.51
1:A:338:ILE:HG22	1:A:341:PHE:H	1.78	0.48
1:A:93:LEU:HB3	1:A:96:ILE:HB	1.94	0.48
1:A:462:ASN:HD21	1:A:466:ASP:HB2	1.79	0.47
1:A:119:PHE:HD1	1:A:147:ILE:HG13	1.79	0.47
1:A:478:ILE:HG22	1:A:483:THR:HG22	1.97	0.46
1:A:218:VAL:HG12	1:A:277:ALA:HB3	1.98	0.46
1:A:262:PHE:HA	1:A:265:ILE:HD12	1.99	0.45
1:A:187:THR:HG22	1:B:188:ARG:HH22	1.82	0.45
2:A:601:HVG:O17	2:A:601:HVG:C2	2.61	0.45
1:B:227:TYR:CD1	2:B:601:HVG:C10	3.01	0.43
1:B:227:TYR:CE1	2:B:601:HVG:C10	3.02	0.43
1:B:443:LEU:HD11	1:B:447:ARG:HH21	1.83	0.43
1:B:479:THR:HB	1:B:482:SER:HB3	1.99	0.43
1:B:227:TYR:CD1	2:B:601:HVG:C9	3.02	0.42
1:A:46:ILE:HD13	1:A:416:LEU:HD22	2.02	0.42
1:A:77:GLU:HG3	1:A:344:TYR:HE2	1.85	0.41
1:A:315:ILE:HG13	1:A:315:ILE:H	1.73	0.41
1:A:364:GLU:HA	1:A:369:CYS:HB3	2.03	0.41
1:A:223:SER:HB2	1:A:282:ALA:HA	2.02	0.40
1:B:369:CYS:HB3	1:B:382:LYS:HE2	2.04	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	427/523 (82%)	405 (95%)	20 (5%)	2 (0%)	29	64
1	B	439/523 (84%)	409 (93%)	23 (5%)	7 (2%)	9	36
All	All	866/1046 (83%)	814 (94%)	43 (5%)	9 (1%)	15	48

All (9) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	60	ARG
1	B	60	ARG
1	B	469	GLY
1	A	454	SER
1	B	380	HIS
1	B	470	ARG
1	B	379	SER
1	B	436	THR
1	B	454	SER

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	339/441 (77%)	338 (100%)	1 (0%)	92	97
1	B	340/441 (77%)	338 (99%)	2 (1%)	86	94
All	All	679/882 (77%)	676 (100%)	3 (0%)	91	96

All (3) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	145	ASP
1	B	335	ARG
1	B	449	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (2) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	452	ASN
1	B	321	GLN

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 ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

Of 4 ligands modelled in this entry, 2 are monoatomic - leaving 2 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	$\# Z > 2$
2	HVG	B	601	-	9,17,17	1.31	1 (11%)	9,24,24	1.01	0
2	HVG	A	601	-	9,17,17	1.22	1 (11%)	9,24,24	0.94	0

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
2	HVG	B	601	-	-	0/4/16/16	0/1/1/1
2	HVG	A	601	-	-	0/4/16/16	0/1/1/1

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	601	HVG	C6-C10	-3.02	1.49	1.52
2	A	601	HVG	C6-C10	-3.00	1.49	1.52

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

2 monomers are involved in 7 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	B	601	HVG	5	0
2	A	601	HVG	2	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	435/523 (83%)	0.37	24 (5%)	25 15	48, 66, 93, 105	0
1	B	447/523 (85%)	0.36	22 (4%)	29 18	43, 72, 98, 109	0
All	All	882/1046 (84%)	0.37	46 (5%)	27 17	43, 68, 96, 109	0

All (46) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	243	GLY	3.9
1	A	61	GLY	3.8
1	B	490	HIS	3.6
1	A	259	PRO	3.4
1	B	496	HIS	3.3
1	B	448	ALA	3.3
1	B	482	SER	3.2
1	B	428	ILE	3.2
1	B	492	THR	3.2
1	B	61	GLY	3.1
1	B	273	PRO	3.0
1	A	385	THR	2.9
1	A	90	PRO	2.9
1	A	428	ILE	2.9
1	A	62	VAL	2.7
1	B	376	LYS	2.6
1	B	316	ALA	2.6
1	A	243	GLY	2.5
1	B	481	LYS	2.4
1	A	343	ARG	2.4
1	A	478	ILE	2.4
1	B	246	SER	2.4
1	A	241	GLU	2.4
1	B	343	ARG	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	505	ALA	2.4
1	B	436	THR	2.3
1	A	393	ASP	2.3
1	B	452	ASN	2.3
1	A	273	PRO	2.3
1	A	244	GLY	2.2
1	A	187	THR	2.2
1	A	145	ASP	2.2
1	A	144	PRO	2.2
1	A	237	GLN	2.2
1	A	339	ASP	2.2
1	B	62	VAL	2.2
1	A	371	LEU	2.2
1	B	483	THR	2.2
1	B	504	TRP	2.2
1	A	66	GLU	2.2
1	A	94	SER	2.1
1	A	392	ARG	2.1
1	A	121	GLN	2.1
1	B	274	ASN	2.1
1	B	239	SER	2.1
1	B	90	PRO	2.1

6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

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

6.3 Carbohydrates [i](#)

There are no monosaccharides 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. 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	B-factors(Å ²)	Q<0.9
2	HVG	B	601	17/17	0.92	0.25	51,53,54,55	0

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Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(\AA^2)	Q<0.9
2	HVG	A	601	17/17	0.92	0.28	54,54,54,54	0
3	CL	B	602	1/1	0.94	0.21	54,54,54,54	0
3	CL	A	602	1/1	0.98	0.12	46,46,46,46	0

6.5 Other polymers [i](#)

There are no such residues in this entry.